Helical vortex phase in the non-centrosymmetric CePt₃Si

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We consider the role of magnetic fields on the broken inversion superconductor CePt₃Si. We show that upper critical field for a field along the c-axis exhibits a much weaker paramagnetic effect than for a field applied perpendicular to the c-axis. The in-plane paramagnetic effect is strongly reduced by the appearance of helical structure in the order parameter. We find that to get good agreement between theory and recent experimental measurements of H_{c2} , this helical structure is required. We propose a Josephson junction experiment that can be used to detect this helical order. In particular, we predict that Josephson current will exhibit a magnetic interference pattern for a magnetic field applied perpendicular to the junction normal. We also discuss unusual magnetic effects associated with the helical order.

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The recently discovered heavy fermion superconductor CePt₃Si¹ has triggered many experimental and theoretical studies 2,3,4,5,6,7,8,9 . There are two features which have caused this attention: the absence of inversion symmetry; and the comparatively high upper critical magnetic field (H_{c2}) . Broken inversion symmetry (parity) has a pronounced effect on the quasiparticle states through the splitting of the two spin degenerate bands. This influences the superconducting phase, which usually relies on the formation of pairs of electrons in degenerate quasiparticle states with opposite momentum. The availability of such quasiparticle states is usually guaranteed by time reversal and inversion symmetries (parity)^{10,11}. It is relatively easy to remove time reversal symmetry, e.g. by a magnetic field, and the physical consequences of this have been well studied. However, parity is not so straightforwardly manipulated by external fields. Superconductivity in materials without inversion center therefore provides a unique opportunity in this respect.

The large $H_{c2} \approx 4T$ in CePt₃Si^{1,8} implies that the Zeeman splitting must be non-negligible below $T_c = 0.75K$ (the estimated paramagnetic limit is at $H_P \approx 1.2 \text{ T}$). In a magnetic field, this superconductor has to form Cooper pairs under rather odd circumstances. In particular, it is no longer guaranteed that a state with momentum kat the Fermi surface has a degenerate partner at -k. The state k would rather pair with a degenerate state -k+q and in this way generate an inhomogeneous superconducting phase. We argue below that recent H_{c2} measurements⁸ suggest that this is the case in CePt₃Si. These measurements show that, while the upper critical field is basically isotropic close to T_c , a small anisotropy appears at lower temperature⁸ $(H_{c2}^c/H_{c2}^{ab}) = 1.18$ at T=0). The apparent absence of a paramagnetic limit in CePt₃Si can be explained by lack of inversion symmetry even if the pairing has s-wave symmetry 2,12,13 . However, these works indicate that suppression of paramagnetism is very anisotropic and the application of this theory to CePt₃Si would indicate no paramagnetic suppression for the field along the c-axis, but a suppression for the field in-plane $(H_P^{ab} \approx 1.7T)$. The relative lack of anisotropy

in the experimental data is surprising in this context.

In this letter we examine the mixed phase close to the upper critical field. Using the crystal symmetry of CePt₃Si, we show that the high-field superconducting phase has pronounced differences for field-directions parallel and perpendicular to the c-axis. For the field parallel to the c-axis, the paramagnetic limiting is basically absent and the vortex phase is quite conventional. While for the perpendicular field direction, the field can induce a phase which gives rise to an additional phase factor in the many body wavefunction $e^{i\boldsymbol{q}\cdot\boldsymbol{R}}$ with \boldsymbol{q} perpendicular to the applied field: a helical vortex phase. We also propose a Josephson junction experiment that can be used to detect this helical phase factor and discuss a transverse magnetization related to the helical phase.

We use the single particle Hamiltonian

$$\mathcal{H}_{0} = \sum_{\boldsymbol{k},s,s'} \left[\xi_{\boldsymbol{k}} \sigma_{0} + \alpha \boldsymbol{g}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma} + \mu_{B} \boldsymbol{H} \cdot \boldsymbol{\sigma} \right]_{ss'} c_{\boldsymbol{k}s}^{\dagger} c_{\boldsymbol{k}s'} \quad (1)$$

where $c_{{m k}s}^{\dagger}$ ($c_{{m k}s}$) creates (annihilates) an electron with momentum ${m k}$ and spin s. The band energy $\xi_{{m k}}=\epsilon_{{m k}}-\mu$ is measured relative to the chemical potential $\mu,\ \alpha g_{{m k}}\cdot \sigma$ introduces the antisymmetric spin-orbit coupling with α as a coupling constant (we set $\langle g_{{m k}}^2 \rangle = 1$ where $\langle ... \rangle$ is an average over the Fermi surface), and $\mu_B {m B} \cdot \sigma$ gives the Zeeman coupling. The crucial term in Eq. 1 is $\alpha g_{{m k}}\cdot \sigma,$ which is only permitted when inversion symmetry is broken ($g_{{m k}}$ satisfies $g_{{m k}}=-g_{-{m k}}$ due to time reversal symmetry). This term destroys the usual two-fold spin degeneracy of the bands by splitting the band into two spin-dependent parts with energies $E_{{m k},\pm}=\xi_{{m k}}\pm\alpha |g_{{m k}}|$. The spinors are determined by the orientation of the corresponding $g_{{m k}}$. The general pairing interaction is

$$\mathcal{H}_{pair} = \frac{1}{2} \sum_{\boldsymbol{k}, \boldsymbol{k}, \boldsymbol{q}, s_{i}} V(\boldsymbol{k}, \boldsymbol{k}') \times c_{\boldsymbol{k} + \boldsymbol{q}/2, s_{1}}^{\dagger} c_{-\boldsymbol{k} + \boldsymbol{q}/2, s_{2}}^{\dagger} c_{-\boldsymbol{k}' + \boldsymbol{q}/2, s_{2}}^{\dagger} c_{\boldsymbol{k}' + \boldsymbol{q}/2, s_{1}}^{\dagger},$$
(2)

expressed in the usual spin basis. We will work in the large α limit so that the pairing problem becomes a real

two-band problem in the diagonal spinor (\pm) basis. To find the pairing interaction in the \pm basis, we diagonalize the single particle Hamiltonian after which the two-band pairing interaction, for $\boldsymbol{H}=0$, is written in spinor form as

$$V = \frac{1}{2}V(\mathbf{k}, \mathbf{k}') \begin{pmatrix} e^{i\phi_-} A_+ & e^{-i\phi_+} A_- \\ e^{i\phi_+} A_- & e^{-i\phi_-} A_+ \end{pmatrix}$$
(3)

where $\phi_{\pm} = \phi_{\mathbf{k}} \pm \phi_{\mathbf{k}'}$ and $A_{\pm} = (1 \pm \hat{\mathbf{g}}_{\mathbf{k}} \cdot \hat{\mathbf{g}}_{\mathbf{k}'})$ where we have taken $\mathbf{g}_{\mathbf{k}} = |\mathbf{g}_{\mathbf{k}}| (\sin \theta_{\mathbf{k}} \cos \phi_{\mathbf{k}}, \sin \theta_{\mathbf{k}} \sin \phi_{\mathbf{k}}, \cos \theta_{\mathbf{k}})$. Note that even for a spatially isotropic interaction, the

two-band solution has both a spin-triplet and a spinsinglet gap function when $\alpha \neq 0$ (this is a consequence of the broken parity symmetry¹³). We will consider the limit $\alpha >> \mu_B H$ and keep only terms up to order $\mu_B H/\alpha$ (a good approximation for CePt₃Si). We restrict ourselves to choices of $V(\mathbf{k}, \mathbf{k}')$ that corresponds to spinsinglet pairing in the $\alpha = 0$ limit. This restriction allows us to use Eq. 3, even if $\mathbf{H} \neq 0$, which considerably simplifies the notation.

With the two band pairing interaction of Eq. 3, the linearized gap equation becomes

$$\Delta_{\alpha}(\mathbf{k}, \mathbf{q}) = -T \sum_{n, \mathbf{k}'} \sum_{\beta} V_{\alpha, \beta}(\mathbf{k}, \mathbf{k}') G_{\beta}^{0}(\mathbf{k}' + \mathbf{q}/2, i\omega_{n}) G_{\beta}^{0}(-\mathbf{k}' + \mathbf{q}/2, -i\omega_{n}) \Delta_{\beta}(\mathbf{k}', \mathbf{q})$$
(4)

where $G_{\pm}^{0}(\mathbf{k}, i\omega_{n}) = [i\omega_{n} + \xi_{\mathbf{k}} \pm \alpha |\mathbf{g}_{\mathbf{k}}|]^{-1}$. Setting $\Delta_{+}(\mathbf{k}, \mathbf{q}) = e^{i\phi}\mathbf{k}\tilde{\Delta}_{+}(\mathbf{k}, \mathbf{q})$ and $\Delta_{-}(\mathbf{k}, \mathbf{q}) = -e^{-i\phi}\mathbf{k}\tilde{\Delta}_{-}(\mathbf{k}, \mathbf{q})$ results in the simplified two-band equation with the interaction

$$V = V(\mathbf{k}, \mathbf{k}')(\sigma_0 - \sigma_x)/2.$$
 (5)

The factors \hat{g} in Eq. 3 do not appear because of Pauli exclusion and the assumed singlet form of V(k, k') in the

 $\alpha=0$ limit. We denote the density of states on the two Fermi surfaces by $N_+=N\cos^2(\delta/2)$ and $N_-=N\sin^2(\delta/2)$. We can write $\tilde{\Delta}_{\alpha}(\boldsymbol{k},\boldsymbol{q})=\psi_{\Gamma,\alpha}(\boldsymbol{q})f_{\Gamma}(\boldsymbol{k})$, where Eq. 5 implies that $\psi_{\Gamma,+}(\boldsymbol{q})+\psi_{\Gamma,-}(\boldsymbol{q})=0$. With $\psi_{\Gamma,+}(\boldsymbol{q})=-\psi_{\Gamma,-}(\boldsymbol{q})=\psi(\boldsymbol{q})$ and the proper Fourier transform of the gap equation keeping gauge invariance, we find the following equation determining the upper critical field

$$\Psi(\boldsymbol{R}) \frac{\ln t}{t} = \int_0^\infty \frac{du}{\sinh(tu)} \left\langle |f_{\Gamma}(\boldsymbol{k})|^2 [\cos(\tilde{\mu}\tilde{\boldsymbol{H}} \cdot \hat{\boldsymbol{g}}u) + i\cos\delta\sin(\tilde{\mu}\tilde{\boldsymbol{H}} \cdot \hat{\boldsymbol{g}}u)] e^{-|\hat{v}_{\perp}|^2 \tilde{H}u^2/2} e^{\hat{v}_{+}\Pi_{+}\sqrt{\tilde{H}}u} e^{-\hat{v}_{-}\Pi_{-}\sqrt{\tilde{H}}u} - 1 \right\rangle \Psi(\boldsymbol{R})$$

where $t = T/T_c$, $\tilde{H} = Hv_F^2/(2\pi\Phi_0T_c^2)$, $\tilde{\mu} = \mu_B 2T_c\Phi_0/v_F^2$, $v_F^2 = \langle v_\perp^2 \rangle = \langle v_1^2 + v_2^2 \rangle$, $v_\pm = (v_1 \pm iv_2)/\sqrt{2}$, $v_{1,2}$ are components of the Fermi velocity perpendicular to the magnetic field, $\Pi^\pm = (D_1 \mp iD_2)l_H/\sqrt{2}$, $l_H^2 = \Phi_0/(2\pi H)$, and $D_i = -i\partial_i - 2eA_i/c$. The upper critical field H_{c2} is found by expanding $\Psi(\mathbf{R}) = \sum_n a_n \phi_n(\mathbf{R})$ ($\phi_n(\mathbf{R})$ are the usual Landau levels).

In the following we take a spherical Fermi surface. For CePt₃Si this will not be the case, but the overall geometry of the Fermi surface does not qualitatively change our results. We also take $g_{\mathbf{k}} = \sqrt{3/2}(-k_y, k_x, 0)$ as the lowest order term in k allowed by symmetry and consider the case $V(\mathbf{k}, \mathbf{k}') = V_0$ for isotropic s-wave pairing. Our re-

sults will hold for any pairing symmetry as the Ginzburg Landau (GL) theory discussed later will demonstrate.

For the field along the c-axis, $\hat{g} \cdot H = 0$ so H_{c2} is independent of the Zeeman field and there is no paramagnetic effect (note that in principle there can be a paramagnetic effect since there are g_k allowed by symmetry that contain a g_z component⁷, however such terms are expected to be small). The solution of the upper critical field problem is identical to that carried out by Helfand and Werthamer¹⁴ and is plotted in Fig. 1. However, for fields perpendicular to the c-axis unusual properties occur, which can be best illustrated by a GL theory with free energy density

$$f = -a|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \frac{1}{2m}|\mathbf{D}\Psi|^2 + \frac{1}{2m_c}|D_z\Psi|^2 + \epsilon \mathbf{n} \cdot \mathbf{B} \times [\Psi(\mathbf{D}\Psi)^* + \Psi^*(\mathbf{D}\Psi)] + \frac{\mathbf{B}^2}{8\pi}$$
(6)

where $a = a_0(T_c^0 - T)$, $\boldsymbol{D} = (D_x, D_y)$, \boldsymbol{n} is the unit vector

oriented along the c-axis, and $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$. Eq. 6 applies

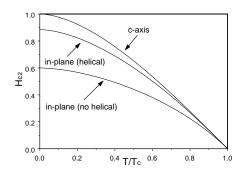


FIG. 1: Upper critical fields for CePt₃Si with fields along the c-axis and in the plane. The actual in-plane H_{c2} will lie between the two extremes shown. The effect of the helical order on H_{c2} can be quite pronounced. These calculations are for $\alpha_M = 3$.

to all possible pairing symmetries with a single complex order parameter, as discussed also by Samokhin⁷. The lack of inversion symmetry allows for the existence of the term proportional to ϵ (for a discussion of other related terms see Ref. 15). This term induces a spatially modulated solution in a uniform magnetic field. The GL equation for the order parameter $\tilde{\Psi}(\mathbf{R}) = e^{i\mathbf{q}\cdot\mathbf{R}}\Psi(\mathbf{R})$ in a field is identical to the zero- ϵ GL equation with $\Psi(\mathbf{R})$, where

$$q = -2m\epsilon \ \boldsymbol{n} \times \boldsymbol{B} \tag{7}$$

(a microscopic expressions for q is given below). Consequently, the upper critical field solution in the GL limit is $\Psi(\mathbf{R}) = \phi_0(\mathbf{R})e^{i\mathbf{q}\cdot\mathbf{R}}$. We call this phase the *helical vortex phase*. The helical order coincides with an increase in the upper critical field $(\mathbf{B} = \mathbf{H})$:

$$T_c(\mathbf{H}) = T_c - \frac{\pi H}{\Phi_0 \sqrt{m m_c} a_0} + \frac{m \epsilon^2 (\mathbf{n} \times \mathbf{H})^2}{2a_0}.$$
 (8)

The expression for the supercurrent density is

$$J = c\nabla \times [B - 4\pi m]/4\pi = J_0 + 4\epsilon e(n \times B)|\Psi|^2$$
 (9)

where J_0 is the usual supercurrent density in the GL limit and $m = \frac{\epsilon m}{e} n \times J_0$ is the magnetization due to the ϵ term Eq. 6. The usual boundary condition on the order parameter is given by J=0 through the boundary. The appearance of m in Eq. 9 is highly unusual in GL theory and has some consequences that are discussed later. Note that if $|\Psi|$ and B are spatially uniform then J=0 for q given by Eq. 7; the helical phase carries no current. The possibility of this helical order has been raised in the context of thin film or interface superconductivity where the vector potential can be neglected 16,17,18 . As discussed below, we find here that it can play a very important role in the vortex phase.

The increase in H_{c2} due to the appearance of the helical plays an important role in the microscopic theory. Since

 $\mathbf{q} \cdot \mathbf{H} = 0$, we can expand $\phi_0(\mathbf{R})e^{i\mathbf{q} \cdot \mathbf{R}} = \sum_n b_n(q)\phi_n(\mathbf{R})$ where $b_n = (iql_H)^n e^{-(ql_H)^2/4}/\sqrt{2^n n!}$. Our numerical microscopic solution has this form and near T_c we find,

$$q = 2\mu_B H \cos \delta \frac{\langle \hat{\boldsymbol{g}}(\boldsymbol{k}) \cdot \hat{\boldsymbol{x}} v_{F,y}(\boldsymbol{k}) | f_{\Gamma}(\boldsymbol{k})|^2 \rangle}{\langle v_{F,y}^2 | f_{\Gamma}(\boldsymbol{k})|^2 \rangle}, \qquad (10)$$

for $f_{\Gamma}(\mathbf{k}) = 1$ this gives $ql_H = 0.373\alpha_M \cos \delta \sqrt{H/H_{c2}^0}$ where $\alpha_M = \sqrt{2}H_{c2}^0/H_P$ is the Maki parameter, H_{c2}^0 is the upper critical field for $\mu_B = 0$ (this coincides with the H_{c2} for the field along the c-axis), and $H_P =$ $\Delta/(\mu_B\sqrt{2})$. For $f_{\Gamma}(\mathbf{k})=k_x^2-k_y^2$, Eq. 10 gives $ql_H=$ $0.418\alpha_M\cos\delta\sqrt{H/H_{c2}^0}$. The enhancement of H_{c2} due to the helical order can be substantial as Fig. 1 shows. Our numerical results show ql_H can be larger than one, which implies that the helical wavelength becomes less than the spacing between vortices. Fig. 1 is for $\alpha_M = 3$ which is slightly smaller than $\alpha_M = 3.8$ that follows from the measurements of Ref. 8. The helical order changes with varying $\cos \delta$. For $\cos \delta = 0$ the density of states are the same on both Fermi surfaces and no helical order appears (labelled 'in-plane (no helical)' in Fig.1); while for $\cos \delta = 1$, ql_H is maximum (this corresponds to the curve labelled 'in-plane (helical)' in Fig. 1). For all other possible values of $\cos \delta$, the H_{c2} curve lies between these two extremes. The limit $\cos \delta = 1$ is unlikely since this implies that the density of states of one of the two bands vanishes. However, if the elements of the pairing interaction $V_{\alpha,\beta}$ in Eq. 5 are different in magnitude from each other, then a large ql_H can still arise for $\cos \delta = 0$.

Comparing our result with the H_{c2} -measurement by Yasuda et al.⁸ for CePt₃Si, we find that only taking the effect of the spin-orbit coupling into account would not account for the relatively large value of the in-plane $H_{c2} \approx 2.8T$) at T=0. Here, paramagnetic limiting should reduce the value to below 2 T. We can, however, explain the increased H_{c2} by including the helicity.

We have also examined the behavior of the Abrikosov parameter $\beta_A = \langle |\Psi(\boldsymbol{R})|^4 \rangle / \langle |\Psi(\boldsymbol{R})|^2 \rangle^2$ in connection with the possible vortex lattice structures. We find a possible structural transition from a stretched hexagonal lattice at high temperatures to a stretched square lattice at low temperatures. The origin of this transition is related to the two-dimensional inhomogeneous state discussed in Refs. 18,19,20. Note that the helical order discussed above is distinct from that discussed in these works. The physics discussed in Refs. 18,19 does not play a significant role in CePt₃Si because the value of α_M is too small. However, if $\alpha_M >> 1$ then the vortex physics becomes very exotic.

We have not discussed the direct experimental verification of the helical phase. Since helicity of the order parameter is related to its phase, an interference experiment based on the Josephson effect would provide the most reliable test. Here we propose to consider a Josephson junction between two thin film superconductors (Fig. 2), one (1) with and the other (2) without inversion symmetry (for CePt₃Si the c-axis is perpendicular to the film).

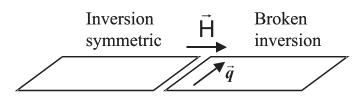


FIG. 2: Josephson junction geometry for the observation of a helical phase.

For a magnetic field applied in the plane of the film per-pendicular to the junction and with the superconductor (2) is oriented so that the helicity q is perpendicular to the field; we find this gives rise to an interference effect analogous to the standard Fraunhofer pattern. For this experiment, the film must be sufficiently thin that the magnetic field and the magnitude of the order parameter are spatially uniform.

To illustrate this, consider the following free energy of the junction

$$H_J = -t \int dx [\Psi_1(\mathbf{R}) \Psi_2^*(\mathbf{R}) + c.c.]$$
 (11)

where the integral is along the junction. The resulting Josephson current is

$$I_J = Im \left[t \int dx \Psi_1(\mathbf{R}) \Psi_2^*(\mathbf{R}) \right]$$
 (12)

Setting the junction length equal to 2L, and integrating yields a maximum Josephson current of

$$I_J = 2t|\Psi_1^0||\Psi_2^0| \frac{|\sin(qL)|}{|qL|}$$
 (13)

This, combined with the result of the microscopic theory near T_c (for an isotropic interaction) that $qL=2.4\cos\delta\alpha_M H\xi_0 L/\Phi_0$ (where $\xi_0=0.18v_F/T_c$) demonstrates that the Josephson current will display an interference pattern for a field perpendicular to the junction. Note that in the usual case the Fraunhofer pattern would be observed for a magnetic field perpendicular to the thin film. Furthermore, for a sufficiently large in-plane field,

so that |qL| >> 1 (which implies $I_J \approx 0$), the arguments of Ref. 21 imply that the application of an additional magnetic field along the surface normal will lead to an asymmetric Fraunhofer pattern.

A less direct probe of the helical order is to look for the related transverse magnetization that appears in Eq. 9. There are two situations for which this can be observed. The first is in a thin film with a supercurrent flowing along \hat{x} and a surface normal along \hat{y} . In this case a magnetization will exist along \hat{y} (normal to the film). This situation is a generalization of an experiment originally proposed by Edelstein²². We estimate $|\mathbf{m}| = \frac{3\pi}{4}\cos\delta n_s \mu_B v_s/v_F \sim 0.02$ Gauss assuming $v_s/v_F = 2 \times 10^{-4}$, $\cos\delta = 1/3$, and $n_s = 1 \times 10^{28}$ m⁻³. The second is in the vortex lattice phase for a field applied along the c-axis. In this case, a calculation valid near H_{c2} gives $\mathbf{m} = \frac{\epsilon m}{e} \mathbf{n} \times \mathbf{J}_0$, where \mathbf{J}_0 is the usual supercurrent for the Abrikosov vortex lattice. Near the vortex core, \mathbf{m} is directed radially outward, perpendicular to the applied field.

We have considered the role of magnetic fields on the non-centrosymmetric superconductor CePt₃Si. Using a two-band theory with a Rashba spin-orbit interaction, we have shown that the upper critical field for the field along the c-axis behaves as if it would in a conventional superconductor independent of the paramagnetic (Zeeman) field. We have further shown that while there is a paramagnetic limiting effect for magnetic fields applied in the basal plane, this effect can be strongly reduced by the appearance of a helical order. Our theory agrees with the experimental measurements of H_{c2} , despite a relatively strong Zeeman field, provided this helical order exists. Finally, we have proposed a Josephson junction experiment that can unambiguously identify the helical order and discussed the appearance of a transverse magnetization related to the helical order.

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